

chain nodes:

12

ring nodes:

1 2 3 4 5 6 8 9 10 11

ring bonds:

1-3 1-2 1-11 2-6 2-8 3-4 4-5 5-6 8-9 9-10 10-11

exact/norm bonds:

1-3 2-6 3-4 4-5 5-6

normalized bonds:

1-2 1-11 2-8 8-9 9-10 10-11

G1:CI,F,CF2,CF3,CN,O

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:CLAS\$13:Atom